Project Title

Validated, Multi-Scale Molecular Dynamics Simulations to Predict the Thermophysical Properties of Molten Salts Containing Fuel, Fission, and Corrosion Products

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ABSTRACT:

Predicting the thermophysical properties of molten salts under various conditions is key to the effective design of molten salt reactors (MSRs). Properties such as density, viscosity, heat capacity and thermal conductivity—as well as phase behavior—must be known in order to model flow behavior and heat transfer within a reactor, which is in turn needed for licensing purposes and safe and efficient reactor design. However, physically measuring salt properties under relevant conditions can be difficult. This has led to critical gaps in established properties of molten salts, particularly those containing impurities such as fuel, fission products, and corrosion products. These impurities are likely to alter salt structures and properties as they are consumed and generated within the salt, and MSR models must take these effects into account. Due to the cost and complications associated with physical property measurements of molten salts, an alternative method for predicting thermophysical properties of salts with a variety of impurities is of great importance; molecular dynamics simulations have the potential to provide such a method, with the power to predict molten salt properties across a large parameter space at relatively low cost. This project aims to use integrated first principles and classical molecular dynamics simulations, validated by experimental measurements, to predict thermophysical properties over a wide range of salt compositions and temperatures. We also aim to use the quasi-chemical model, informed by these property measurements, to generate phase diagrams for salt composition.

The specific object of the project is to:

(1) use first principles molecular dynamics (FPMD) based on density functional theory (DFT) to predict the short-range structure and speciation of molten salts containing fuel, corrosion products, and fission products
(2) develop classical molecular dynamics (CMD) potentials for these systems by fitting forces generated by DFT
(3) collect experimental measurements of thermophysical properties (density, heat capacity, thermal conductivity) to expand and validate predictions from MD
(4) use CMD to predict properties (density, heat capacity, thermal conductivity, viscosity) across a wide range of temperatures and compositions, enabling broad models of salt properties at a lower cost than with experimental measurements alone
(5) develop property correlations from experimental and simulated property data